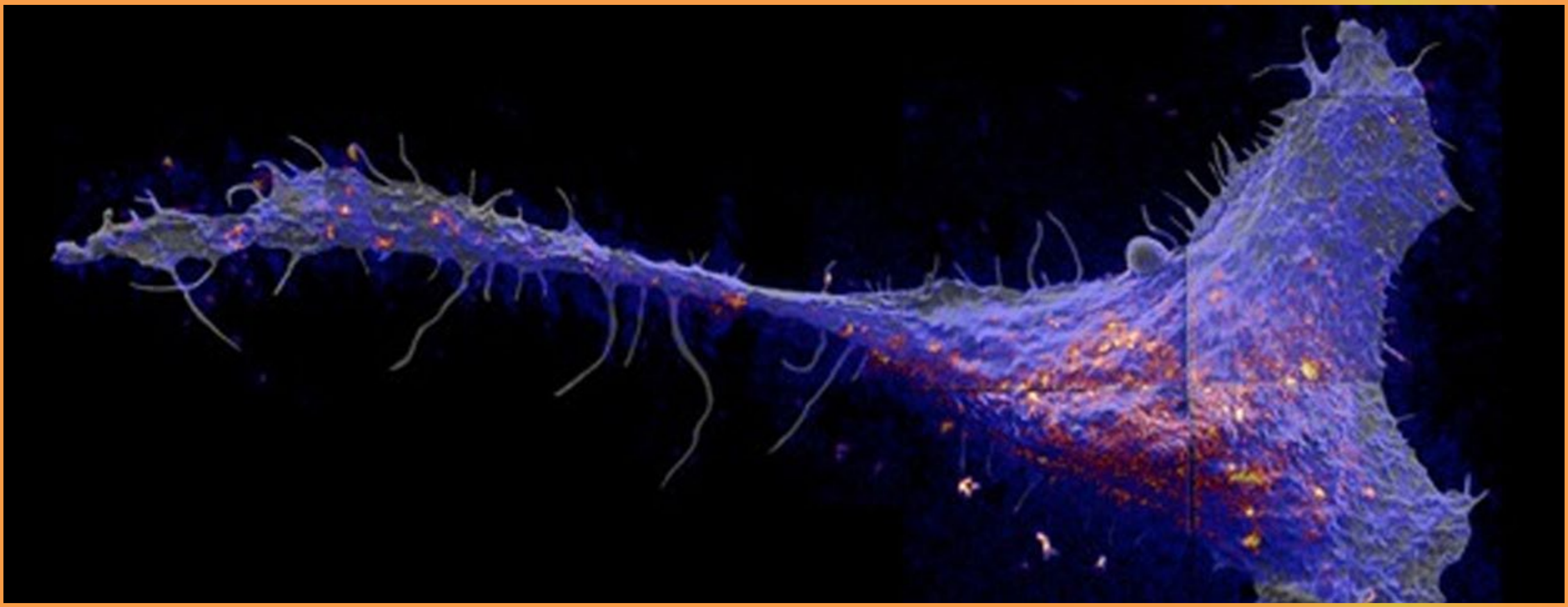
Science and Technology UPDATE

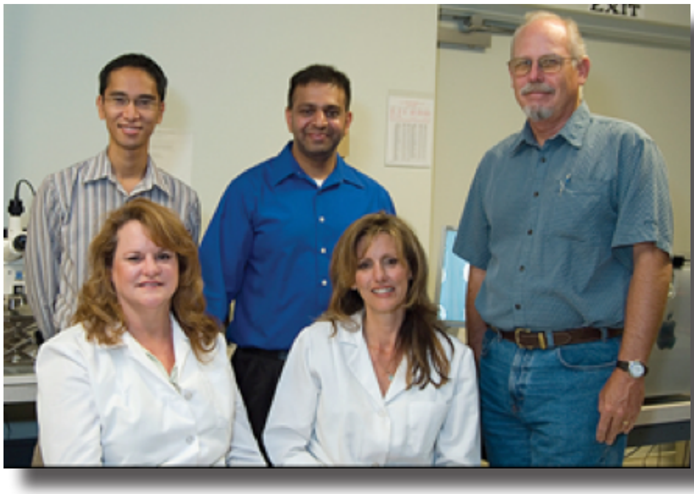
January/February 2013



Science on a Mission

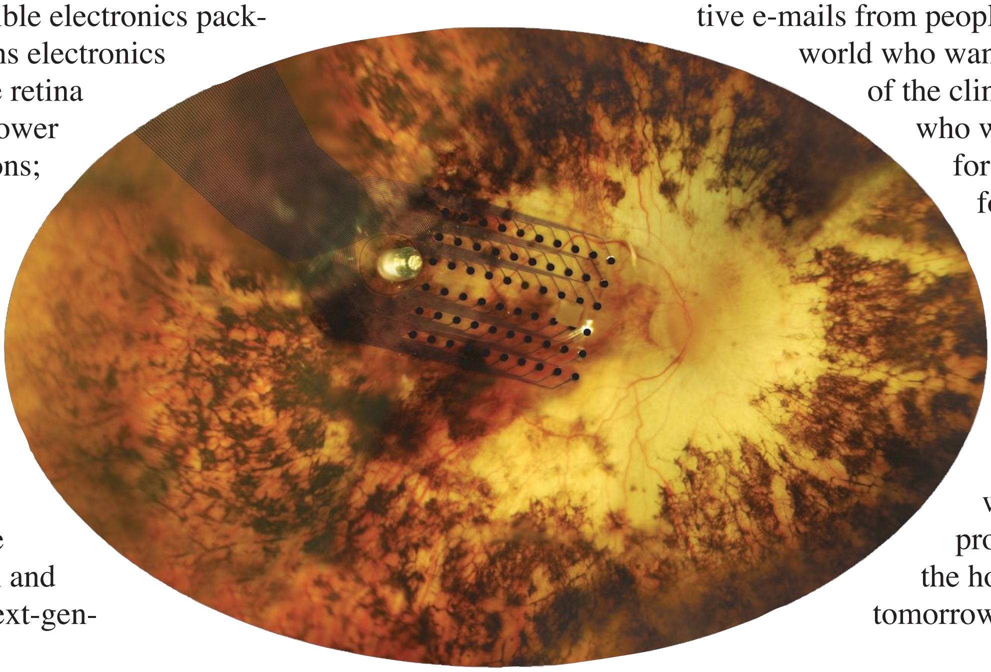
LLNL-MI-630012

ARTIFICIAL RETINA APPROVED BY FDA



In February, DOE **announced** that the retinal prosthesis—or "bionic eye"—that represents a decade of revolutionary DOE-supported research became the first ever to be approved by the FDA. The prosthesis was approved for blind persons with end-stage retinitis pigmentosa, a disease that affects 1 in 4,000 people in the United States. LLNL engineers played a key role in the project by developing the microelectrode array for the prosthesis, among other work. LDRD **support** at Livermore came in the form of a project to develop technologies for smart biodetection systems, of which the artificial retina was an unexpected application. The newly approved retinal device will be manufactured and sold by California's Second Sight Medical Products under the name **Argus II** Retinal Prosthesis System.

The LLNL team contributed three major components to the artificial retina program: (1) the thin-film electrode array, which contains the neural electrodes; (2) the biocompatible electronics package, which contains electronics for stimulating the retina and for wireless power and communications; and (3) an ocular surgical tool that will enable the replacement of the thin-film electrode array. In addition, Lawrence Livermore was responsible for the system integration and assembly of the next-generation artificial retina system. Livermore's **team**—in the photo (front row, left to right) Julie Hamilton and Terri Delima and (back row, left to right) Phillipe Tabada, Satinderpall Pannu, and William Benett—was led by Satinderpall, who states, "The team was very passionate about this project because there is such a need for a device like this. While we were developing the technology, we received a lot of plaintive e-mails from people around the world who wanted to be a part of the clinical trials or who were just looking for a ray of hope for themselves or their children. It is most gratifying to see this device finally become available to the people who need it and provide them with the hope of a better tomorrow."



A bulletin of achievements at Lawrence Livermore National Laboratory.
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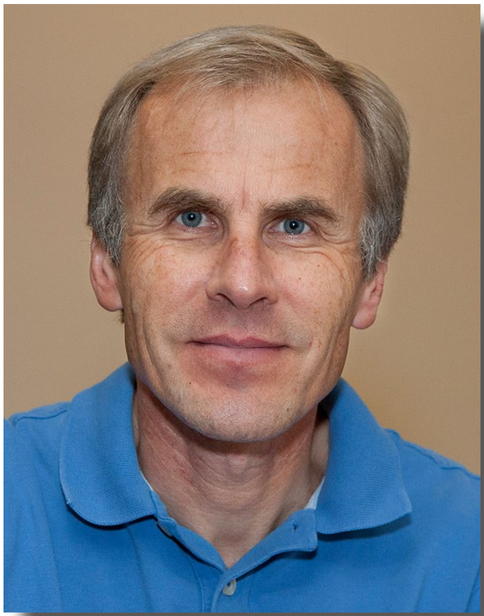
About the Cover

NanoSIMS data, combined with secondary electron images, indicate local elevations in the abundance of sphingolipids in a cell membrane. See "NanoSIMS reveals surprise about cell membrane lipids," on page 12.

NASA Award for Work on Solar Dynamics Observatory

Regina Soufli and her colleagues on the Solar Dynamics Observatory (SDO) Science Investigation Team have been awarded the 2012 NASA Group Achievement Award for "outstanding designing, building, and operating of the science investigations of the SDO, thus enabling the scientific results and mesmerizing the public." The SDO studies the sun's interior and atmosphere and the sun's impacts on Earth's upper atmosphere and nearby space environment. Regina led a team of LLNL researchers including Jeff Robinson, Eberhard Spiller, Sherry Baker, and Jay Ayers and collaborators from LBNL and other institutions in developing, fabricating, and calibrating the multilayer coatings used on the extreme ultraviolet optics of the SDO's Atmospheric Imaging Assembly, which has already contributed to several groundbreaking discoveries, such as sympathetic solar flares and superhigh-speed solar waves. "They have worked for a decade to build, launch, and run SDO," said NASA SDO project scientist Dean Pesnell. "The spectacular imagery and science we get from SDO are a result of their dedication and hard work." The NASA Group Achievement Award is presented annually to a group of government or nongovernment employees who together have made accomplishments that significantly contribute to NASA's mission.

Physicist Elected APS Fellow



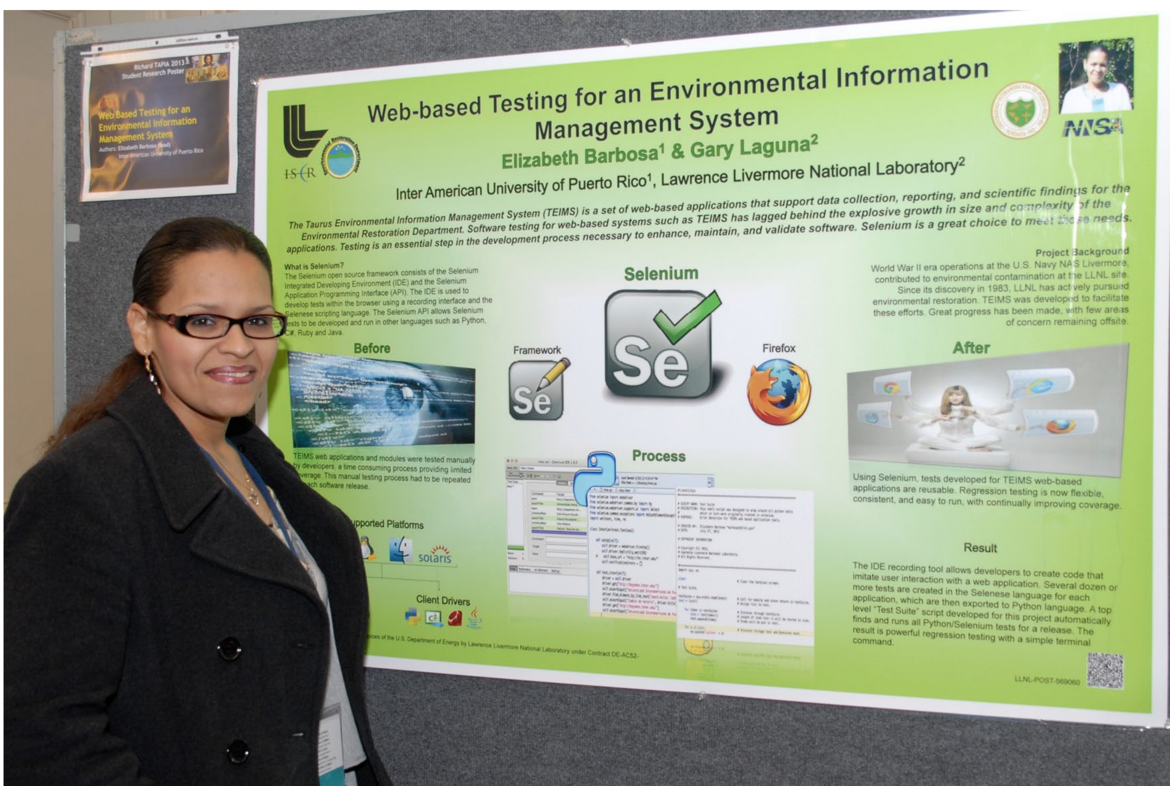
Andris Dimits, a physicist in the Fusion Energy Sciences Program, has been selected as a 2012 fellow of the American Physical Society (APS). Andris was cited in the plasma physics category for "important insights and contributions to the theory and simulation of kinetic turbulent transport in magnetized plasmas, including the effects of self-consistent turbulence-induced velocity shear and Coulomb collisions." He joined LLNL in 1990 and has worked on theory and simulation of magnetized fusion plasmas, hydrodynamic instability and turbulence, and high-energy-density physics, as well as high-order and multilevel Monte Carlo simulation algorithm development. "Working at LLNL has given me the opportunity to work on a variety of stimulating and important problems," Andris said. "It has also provided an excellent base for participation in several very rewarding multi-institutional national and international team collaborations. I feel very fortunate to have been able to work with many dedicated, first-rate scientists, both within LLNL and outside." In the past 25 years, nearly 100 LLNL employees have been elected APS fellows.

ENGINEER ELECTED VICE PRESIDENT OF ASPE

John Taylor has been elected vice president of the American Society for Precision Engineering (ASPE). He will serve in this capacity for calendar year 2013, followed by promotion to president of the society in 2014. John is a charter member of ASPE and currently leads the Precision Systems and Manufacturing Group in Engineering and supports large optics production for NIF. ASPE focuses on many areas of interests that are important in the research, design, development, manufacture, and measurement of high-accuracy components and systems.

STUDENT PRESENTS POSTER AT D.C. DIVERSITY CONFERENCE

Elizabeth Barbosa (photo) was one of four Computation students to participate in the poster session at the 2013 Richard Tapia Diversity in Computing Conference in Washington, D.C. in mid-February. Many LLNL researchers and managers provided support for the **conference**, the largest and most diverse in the gathering's 12-year history. "Playing a high-profile role in the conference gives the Laboratory great visibility and helps us attract top talent from the diverse pool of attendees," said Tony Baylis, a program manager in Computation who has participated in the conference since 2003. A number of conference attendees who came to Livermore, some through student programs, have become full-time employees. This year's **conference** was also attended by U.S. Chief Technical Officer **Todd Park**, who reports to President Obama.



RESEARCHER NAMED OUTSTANDING REVIEWER BY ASCE JOURNAL

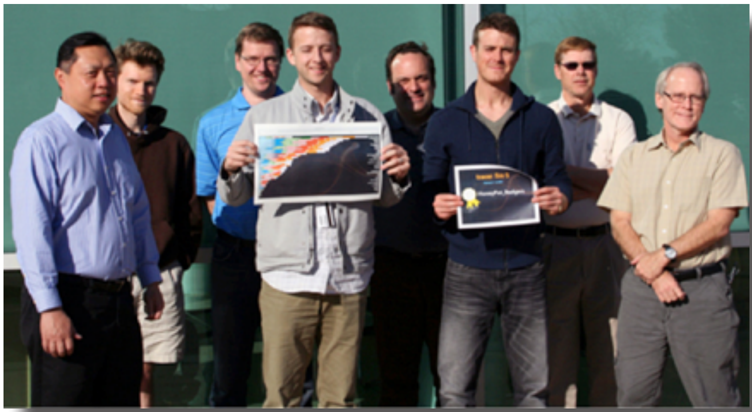
Pengcheng Fu, a **researcher** in the Computational Geosciences Group, has been named an Outstanding Reviewer for 2012 by the *Journal of Materials in Civil Engineering*, which is published by the American Society of Civil Engineers.

NIF SETS RECORD FOR SHOT COUNT AND WAVELENGTH CHANGES

The month of January saw NIF complete a **record 28 laser shots** on targets last month—along with two shots without targets—and a significant increase in experimental flexibility, as the team completed 40 laser wavelength changes, more than double the number in any previous month. Changing the laser wavelength by a few angstroms in different cones of laser beams enables researchers to adjust the amount of energy reaching different areas of the hohlraum targets. The photo shows technician Frank Cebreros testing activation of the target shroud in the NIF cryogenic target positioner in preparation for a January 6 tantalum equation-of-state experiment.

CYBER SECURITY TEAM WINS NNSA-WIDE CHALLENGE

A team of LLNL employees won first place in Tracer FIRE 5, a national laboratory and private sector cyber security competition held in February. The 3-day, around-the-clock online competition was joined by organizations across the United States; LLNL hosted a regional hub at the Livermore Valley Open Campus. Now in its fifth year, Tracer FIRE also includes state-of-the-art training in information security, including network archeology and malware reverse engineering. In the competition that follows, participants measure their capacity against the best in the business from both the Federal government and the private sector. This event seeks to improve

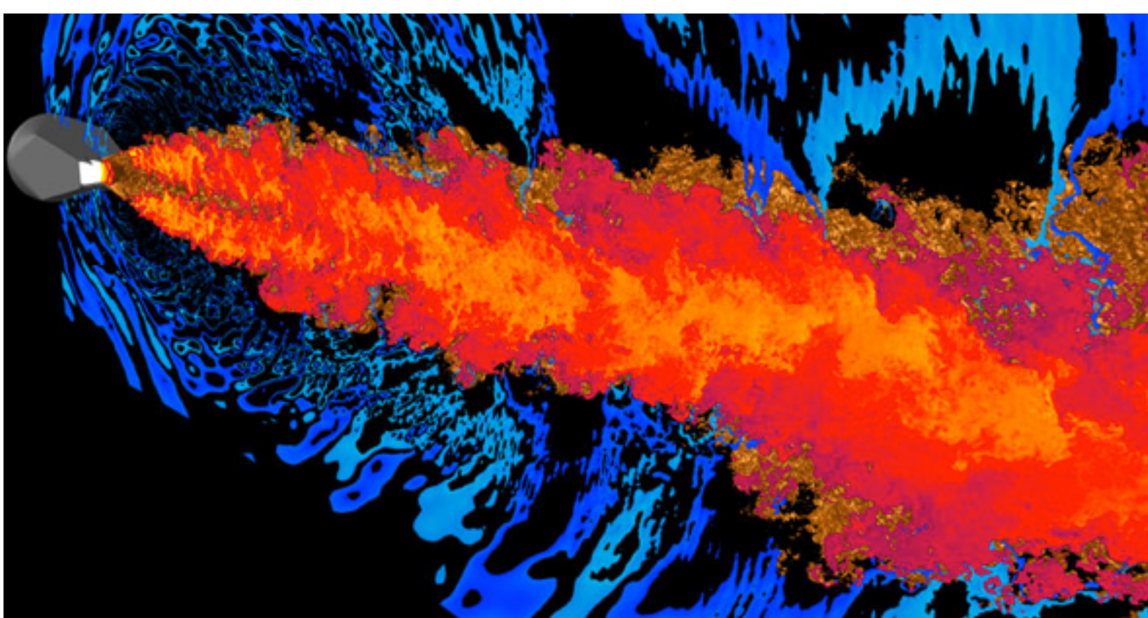


not only the expertise for defending against cyber attacks but also the communication between NNSA sites during such an event. The LLNL team bested teams from Pacific Northwest National Lab and Bechtel Headquarters, among others. Nicknamed the "HoneyPot_Badgers" after a type of cyber security defense and Louisiana State University's former star defensive back, the team consisted of (left to right in photo) Richard Mark, Peter Scheibel, Sergei Nikolaev, Alan Liddeke, Peter Barnes, David Sontheimer, Reggie Hunt, and Allen Sturtevant. Livermore teams have won two of the last four Tracer FIRE events.

SEQUOIA SIMULATION BREAKS MILLION-CORE BARRIER

In a true success story of outside researchers using LLNL's Sequoia Bluegene/Q supercomputer for groundbreaking work, a team from Stanford University's Center for Turbulence Research (CTR) running a simulation on Sequoia set a **new record** in computational science by using more than one million computing cores. (This comes on the heels of two teams **breaking** the 10-petaflop barrier late last year.) The CTR simulation examined a complex fluid dynamics problem—the prediction of noise generated by a supersonic jet engine—to test **nozzle shapes** that could produce less noise than current designs.

Working with NASA's Glenn Research Center and the U.S. Navy, the CTR team seeks to predict how loud an experimental engine will be without having to actually construct a prototype. The image (courtesy of CTR) from the jet noise simulation shows a new design for an engine nozzle (left), with exhaust temperatures in red–orange and the sound field in blue–cyan, indicating how chevron-shaped elements along the nozzle rim enhance turbulent mixing to reduce noise. "These runs represent at least an order-of-magnitude increase in computational power over the largest simulations performed at the Center for Turbulence Research previously," said CTR researcher associate Joseph Nichols. "The implications for predictive science are mind-boggling."



STRATEGIST JOINS PANEL ON SOUTH ASIA NUCLEAR TENSION

Livermore's Neil Joeck joined a **panel discussion** in Washington, D.C., titled "The Stability of Deterrence in South Asia," sponsored by the Carnegie Endowment for International Peace. Neil—whose career includes serving the White House from 2009 to 2011 as National Intelligence Officer for South Asia in the Office of the Director for National Intelligence—touched on the potential for all-out war between India and Pakistan, the possibility of such a conflict escalating to nuclear weapons use, and on the need for re-evaluating strategy for nuclear deterrence in the region in light of developments such as Pakistan's development of theater nuclear weapons and the coming naval deployment by both nations of their nuclear technology and weaponry.

WORKSHOP ON USING NIF TO STUDY INTERIORS OF GIANT PLANETS

Topics ranging from the behavior of hydrogen and helium at extreme densities to "surprises" in planetary physics research were explored at workshop at LLNL last December on using the capabilities of NIF to study the interiors of giant planets. Hosted by LLNL's Rip Collins and UC Berkeley's Raymond Jeanloz, the workshop discussed how the unprecedented temperatures and pressures created by NIF can further researchers' understanding of the physics involved in the creation and evolution of planets. Also discussed was the science of materials subjected to pressures higher than one terapascal (ten million times Earth's atmospheric pressure). Outside organizations represented at the workshop include Caltech, the Carnegie Institution of Washington, the Institute of Shock Physics at Washington State University, and the Centre for Science at Extreme Conditions at the University of Edinburgh.

ATOMIC X-RAY LASER ON "TOP STORIES OF 2012" LIST

The **creation** of the world's first atomic x-ray laser by a team of researchers representing LLNL, the Stanford Linear Accelerator Center, and Colorado State University was ranked 5th by Photonics Media on its list of the **10 most popular stories of 2012** at their biophotonics website Photonics.com. The x-ray laser pulses—the shortest, purest ever created—were generated by aiming the Linac Coherent Light Source at a capsule of neon gas, setting off an avalanche of x-ray emissions. The achievement, which fulfilled a 45-year-old prediction, was announced in a **paper** in *Nature*.

LABORATORY IN APS TOP PHYSICS STORIES OF 2012

Two LLNL achievements in physics were among the **top physics stories** in 2012 as assessed by the American Physical Society. One is the official naming in May 2012 of element number 116 as livermorium (Lv), after the Laboratory. The second achievement is the achieving of the title of "World's Fastest Computer" in June 2012, when Sequoia topped out at 16.2 petaflops.

CO_2-FLUX-MONITORING STATION PLUGS INTO AMERIFLUX NETWORK

A three-meter-tall "eddy flux" tower located at Site 300 and operated by LLNL researcher Sonia Wharton has officially joined the **AmeriFlux** network. Named "Diablo," the tower station collects data on the exchange of CO_2, water, energy, and momentum between the local terrestrial ecosystem and the atmosphere. The station is located at LLNL's Site 300 and has been operating since October 2010. The entire record of data taken by the station is now available online. The AmeriFlux network is a federation of similar micrometeorological sites across North, Central, and South America whose goal is to quantify spatial and temporal variations in carbon storage in plants and soils, and exchanges of carbon, water, and energy in major vegetation types across a range of disturbance histories and climatic conditions in the Americas. The resulting data will advance understanding of processes regulating carbon assimilation, respiration, and storage, and linkages between carbon, water, energy and nitrogen.

LABORATORY VELOCIMETER USED IN SUBCRITICAL EXPERIMENT

When the 27th subcritical experiment was **conducted** at the Nevada National Security Site in December, a new LLNL-developed multiplexed photonic doppler velocimeter (MPDV) was used to measure up to 32 discrete shock wave surface velocities. These and other data were generated for use in the Stockpile Stewardship Program. Said then-NNSA Administrator Tom D'Agostino, "I applaud the work done by the men and women who worked to make this experiment successful. Experiments such as this help deliver President Obama's nuclear security agenda." This was the first such experiment to use the MPDV, which **won an R&D 100 Award** in 2012.

PHYSICIST APPOINTED TO NUCLEAR ADVISORY COMMITTEE

Nuclear physicist Erich Ormand has been asked to serve as a member of the Nuclear Science Advisory Committee (**NSAC**). Chartered under the Federal Advisory Committee Act, NSAC provides official advice on the nation's program for basic nuclear science research to both DOE and the National Science Foundation, which share responsibility for the direction of NSAC, including selecting members and defining meeting agendas.

SOFTWARE PARTNER ACHIEVES DEBUGGING MILESTONE

In a key milestone in its scalability initiative with LLNL, LANL, and Sandia, Rogue Wave Software recently **announced** that its TotalView software successfully debugged a parallel application running on over 700,000 cores on Sequoia. The run was so trouble free that software engineers concluded that the application could have easily used more of Sequoia's 1.5 million nodes. An extreme-scale debugging tool like TotalView is essential to converting mission-critical applications to run on tomorrow's exascale architectures.

COMP LEADER NAMED "PERSON TO WATCH" BY HPCWIRE

HPCwire has **named** Computation Associate Director Dona Crawford as one of its "People to Watch" in 2013. The annual list of 12 influential individuals in high-performance computing (HPC) "pays tribute to an exemplary group of the best and brightest minds of HPC, whose hard work, dedication, and contributions we believe reach beyond the spectrum of high-performance computing and will influence the direction that technology will lead us in 2013 and beyond."

Dona has the distinction of being the first woman to be twice selected for the list, previously appearing in 2002. As part of the profile appearing in HPCwire, Dona named the top five developments in HPC to watch in 2013—power efficiency, the battle between Intel Xeon Phi and graphic processing units, programming languages for "big data" applications, high-bandwidth memories, and industrial engagement.

NIF ACHIEVEMENTS CITED IN NATIONAL ACADEMIES REPORT

A **report** issued by the National Research Council highlights the significant impact of successful development of inertial fusion energy (IFE) and recommends priorities for future research: "The potential benefits of inertial confinement fusion energy (abundant fuel, minimal greenhouse gas emissions, limited high-level radioactive waste requiring long-term disposal) provide a compelling rationale for establishing inertial fusion energy R&D as part of the long-term U.S. energy R&D portfolio."

The report also confirms NIF's role beyond stockpile stewardship, stating that "the National Ignition Facility, designed for stockpile stewardship applications, also is of great potential importance for advancing the technical basis for [IFE] research"; that now is the "appropriate time for the establishment of a national, coordinated, broad-based inertial fusion energy program"; and that "planning should begin for making effective use of [NIF] as one of the major program elements in an assessment of the feasibility of inertial fusion energy." The report also notes unanimity among expert review committees on NIF's potential to achieve ignition, a near-term goal of NIF that would mark the culmination of more than 50 years of effort and is a principal research pillar of the NNSA's mission.

UTILITIES TO TAP INTO LLNL TECHNOLOGY

The California Public Utilities Commission (CPUC) last December approved a 5-year, $150 million agreement between LLNL and three public utilities—Pacific Gas and Electric Company, Southern California Edison Company, and San Diego Gas and Electric Company—that will provide the utilities access to LLNL high-performance computing and other technological capabilities and related domain expertise in engineering and applied science. Under the initiative, called California Energy Systems for the 21st Century (CES-21), the Laboratory will help create the high-tech tools California needs to achieve aggressive renewable energy and greenhouse gas goals and plan for widespread electric transportation. In addition, the initiative also seeks to apply the sophisticated cyber security technology and "smart grid" technology to build a smarter, more secure energy system that will accommodate the growth, prosperity, and value to California rate payers. "The efficiency, reliability and safety of the energy grid, not only in California but across the country, are national security challenges," said Parney Albright, LLNL director. "Lawrence Livermore can bring to bear capabilities in engineering, applied science, computation, and national security that will complement utilities' efforts to build an energy grid for our state's future."

LLNL HOSTS WORKSHOP ON COHERENT NEUTRINO SCATTERING

Last December, LLNL's Advanced Detectors Group, working with Sandia colleagues, held a workshop at the Livermore Valley Open Campus on progress being made towards using neutron spallation and reactor neutrino sources to directly experimentally measure coherent neutrino scattering—first predicted in the 1970s based on the Standard Model of particle physics but which has thus far eluded detection. The workshop brought together 30 experts in coherent scatter detection from universities and national laboratories around the world, and presentations were made on a several detector types and detection schemes. The keynote speakers—theorist Leo Stodolsky from the Technical University of Munich and experimentalist Blas Cabrera from Stanford University—discussed progress in this area, with an emphasis on its natural overlap with dark matter searches and astrophysical investigations of supernovae. The workshop concluded with ideas for possible collaboration, shared use of calibration and neutrino sources, and the outlines of a unified strategy for outreach to sponsors of this work for future investigations.

RESEARCHER HELPS SOLVE ITER SUPERCONDUCTING MAGNET PROBLEM

Nicolai Martovetsky, an LLNL researcher assigned to the U.S. ITER Project Office, was part of the team that developed a "roadmap" for solving a serious problem with the giant superconducting magnets of the ITER fusion reactor. He also participated in subsequent test campaigns and analyses that resolved the problem. At issue were the superconducting cables that make up the central solenoid, a 13.5-meter-high set of coils in the center of the reactor. In late 2010, testing revealed that the cables had a lifetime ten times shorter than required—a problem that threatened the project's scheduled completion in 2020. In response, the ITER team developed a new "short twist pitch" cable design, and samples subjected to testing last November and December showed no signs of appreciable degradation. This significant achievement was **reported** in *Science*.

ENERGY COLLABORATION WITH NDSU FARGO

The Laboratory has signed a memorandum of agreement with the North Dakota State University at Fargo to collaborate on research and development projects involving computational-based modeling and simulation for energy and energy-related applications. Potential research may include enhancing productivity for tightly bound liquid hydrocarbons, such as those found in the Bakken oil shale formation in North Dakota. Other potential research projects could include high-throughput chemical design and development of new, novel materials for energy applications. Said LLNL Director Parney Albright: "We look forward to a close partnership with NDSU faculty, staff, and students, bringing advanced supercomputing to real-world problems in fossil energy and sustainability."

AAAS MEETING SHOWCASES LAB WORK ON FUSION AND SPACE EXPLORATION

The Laboratory underscored its expertise in fusion energy and space exploration at the American Association for the Advancement of Science (AAAS) **2013 Annnual Meeting**, held February 14–18 in Boston. Mike Dunne gave a presentation titled "The Path to Laser Inertial Fusion Energy (LIFE)" as part of a session that explored fusion energy at a turning point, as two approaches—magnetic and inertial fusion—enter new experimental regimes. Debbie Callahan, group leader for inertial fusion target design, gave a talk titled "NIF Program and Ignition Campaign," in which she discussed experimental techniques and results on the path to achieving controlled fusion in the laboratory using the NIF. Finally, LLNL Engineering Director of Mission Development Elizabeth Cantwell presented "Recapturing a Future for Space Exploration: Research for a New Era" in a session that brought together scientists spanning the biological and physical sciences to describe the work they have already done from the space station and the plans and challenges for the next decade.

CRADA FOR BIODETECTOR

The Laboratory has signed a cooperative R&D agreement for the Lawrence Livermore Microbial Detection Array (LLMDA) with Denmark's Statens Serum Institut (SSI), a public enterprise under the Danish Ministry of Health tasked with improving the country's preparedness towards infectious diseases and congenital disorders. An international research organization, SSI has been collaborating with LLNL to use the LLMDA to analyze viral and bacterial infections from human clinical samples. Impressed with LLMDA's speed, efficiency, and cost-effectiveness, SSI will now receive LLMDA software, use it to analyze clinical samples, and provide feedback on effectiveness and accuracy of the microbial detection array, which will enable LLNL to improve the software even further.

TECHNOLOGIES OPTIONED IN ULTRAWIDEBAND IMAGING AND BIO SAMPLE PREPARATION

In February, an LLNL ultrawideband imaging technology was optioned by Underground Imaging Technologies (**UIT**), allowing UIT to license the technology for mapping and imaging underground infrastructure in the construction industry. UIT, a small business located in Orlando, Florida, develops and integrates hardware and software systems to improve the safety, accuracy, and efficiency of designing, building, and managing underground infrastructure. Also in February, LLNL optioned a biological sample-preparation technology to Purigen Biosystems, Inc., a small startup located in Alviso, California.

RESEARCHERS TO HELP STAND UP RARE EARTH RESEARCH CENTER

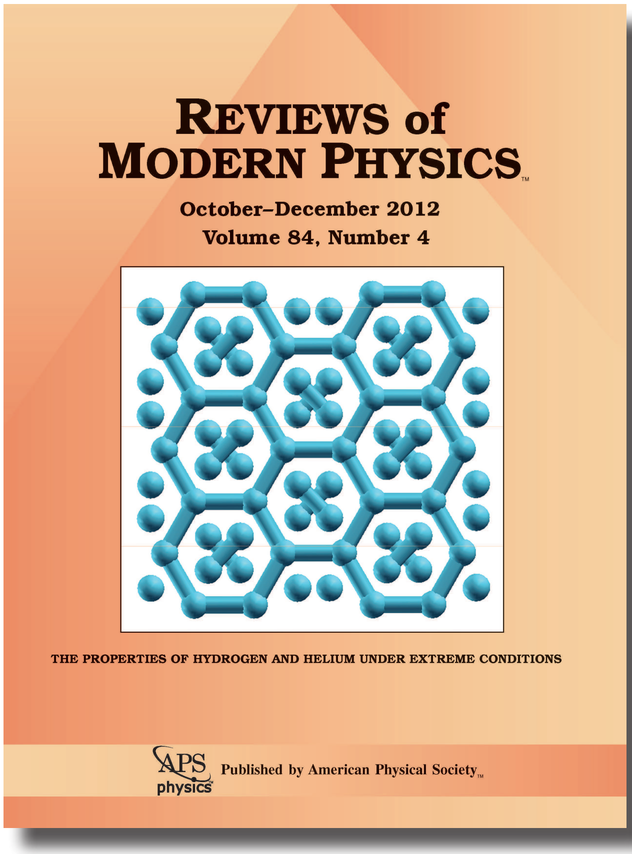
DOE recently **announced** that a team including LLNL researchers will establish a new research center to develop solutions to domestic shortages of rare-earth metals and other materials relevant to national security. The new center, to be named the Critical Materials Institute and sited at Ames Laboratory, "will bring together the best and brightest research minds from universities, national laboratories, and the private sector" to address challenges over the entire material life cycle, from enabling new sources and accelerating material development to improving the efficiency of use. Livermore was one of the four original organizations—the others being Ames, the Colorado School of Mines, and Molycorp. Inc.—on a team that created a national network on the issue, eventually forming a proposal team after the Laboratory hosted the first **U.S.–Japan roundtable** on rare earth elements in 2010.

SCIENTISTS TAPPED TO EDIT NEW JOURNAL

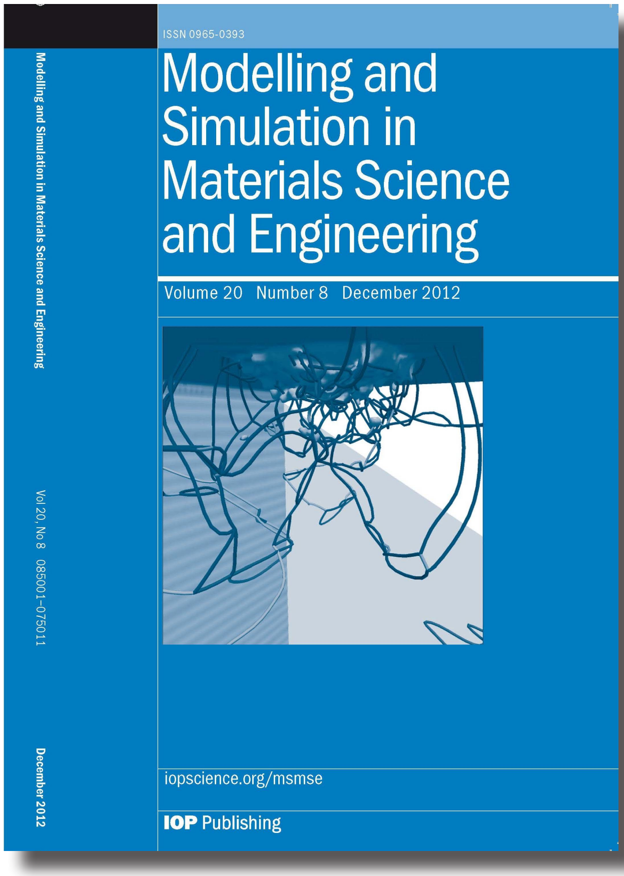
Bradley Hart and Paul Jackson will be editors of the *Journal of Chemical and Biological Defense*, a new peer-reviewed journal in which classified research may be published. The journal will provide a secure forum for the discussion of issues related to sensitive research and investigations into both existing and emerging chemical and biological threats and their countermeasures. Representatives from various agencies, Federal laboratories, and academia founded the journal for the intelligence and classified research and development communities. Access to the journal is through the Army Knowledge Online network.

HYDROGEN AND HELIUM RESEARCH ON *RMP* COVER

The November 13, 2012 issue of *Reviews of Modern Physics* features on its cover the **work** of Miguel Morales-Silva and colleagues at the University of Illinois and Italy's University of L'Aquila on the properties of hydrogen and helium under extreme conditions. Despite being in principle the most simple elements in the universe, hydrogen and helium display remarkably complex properties under extreme conditions of pressure and temperature that have challenged science for decades. Miguel et al.'s paper reviews the state of the art of the advanced computational techniques—particularly density functional theory and quantum Monte Carlo methods—that remain the only tool for predicting properties under conditions not yet experimentally accessible. The paper also discusses phase transition in pure hydrogen, the possibility of a low- or zero-temperature quantum fluid and high-temperature superconductivity, and pure helium and hydrogen–helium mixtures, which are particularly relevant to planetary physics.



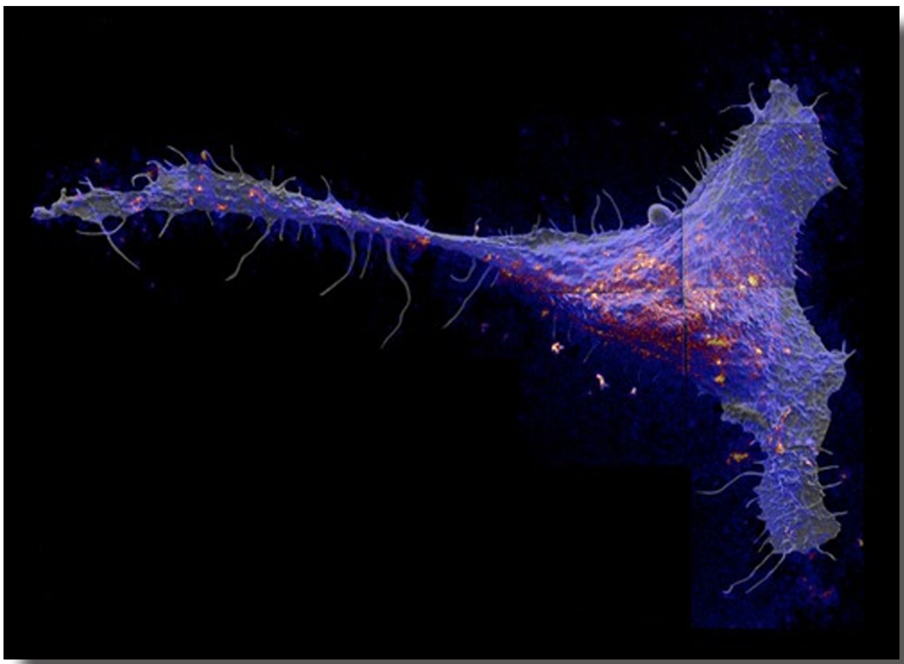
NEW METHOD FOR EXTRACTING DISLOCATION INFORMATION FROM SIMULATIONS



In a **paper** published in the December 2012 issue of *Modelling and Simulation in Materials Science and Engineering* and featured on the issue's cover, former LLNL postdoc Alex Stukowski (now at Technische Universität Darmstadt, Germany) and LLNL colleagues present an automated algorithm that extracts dislocation information from the molecular dynamics simulations of crystalline materials, whose properties are greatly determined by the dislocation that occurs at grain boundaries and other crystal interfaces. The computationally efficient algorithm identifies and indexes dislocations in crystal lattices and interfaces and outputs a representation of the dislocation networks in a form commensurate with classical dislocation theory. The new technique also presents clear advantages over traditional manual methods, which are error-prone, laborious, and, in many cases, unfeasible.

NANOSIMS REVEALS SURPRISE ABOUT CELL MEMBRANE LIPIDS

In a **paper** published in the *Proceedings of the National Academy of Sciences*, LLNL researchers Peter Weber, Ian Hutcheon, and Kevin Carpenter, with colleagues from the University of Illinois and the National Institutes of Health, report on a new method for mapping the distribution of small molecules in a cell membrane. Previous research suggested that lipids in the membrane assemble into patches that differ in composition and help cell membrane proteins carry out basic functions, but understanding was hampered by the inability to directly image their spatial distribution. Using LLNL's nanoscale secondary ion mass spectrometry (nanoSIMS), Peter et al. made high-spatial-resolution images of the distribution of nitrogen-15-labelled sphingolipids, which had been thought to associate with cholesterol to form small domains about 200 nanometers across. The nanoSIMS images revealed that sphingolipids form domains much larger than previously thought, that the 200-nanometer domains cluster together to form micrometer-sized patches, and that domain formation was affected less by cholesterol than by proteins underlying the membrane. These findings fundamentally challenge existing assumptions about how lipids and proteins are organized in the cell membrane, and that data collected with imaging techniques targeting the underlying proteins are not as accurate in representing sphingolipid distribution as previously thought. LLNL's work in this project was funded by the LDRD program. The image combines nanoSIMS data with secondary electron images to visually show local elevations in sphingolipid abundance (red and yellow).

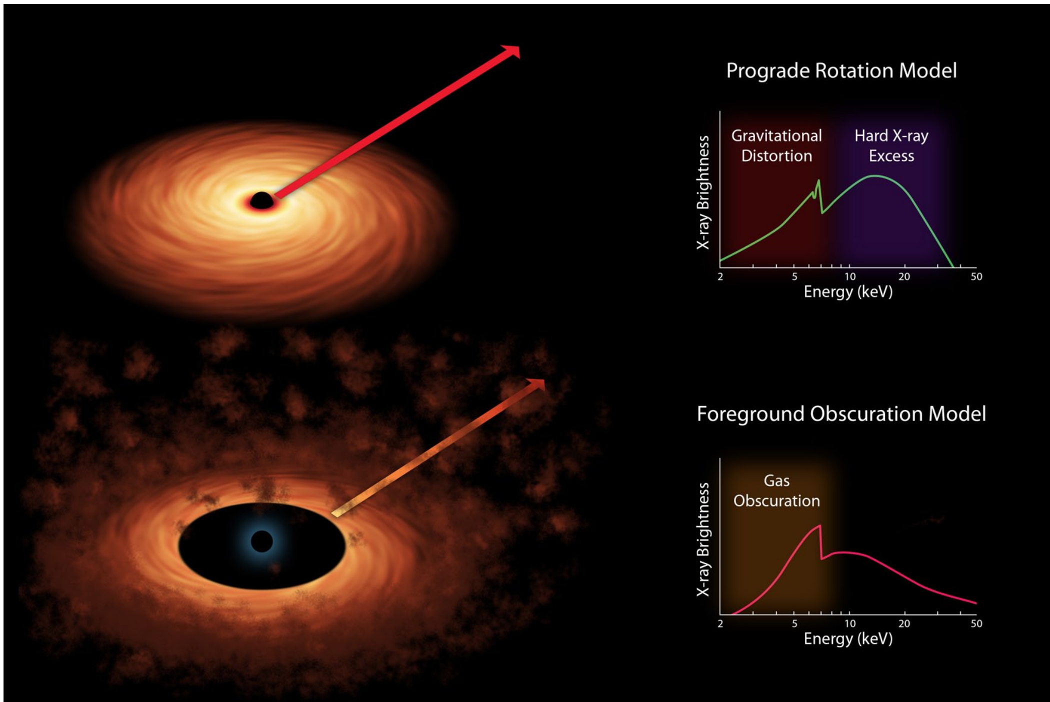


LLNL PAPERS AMONG MOST-DOWNLOADED IN *PHYSICS OF PLASMAS*

Physics of Plasma's 20 **most-downloaded papers** for the month of December 2012 include four by LLNL authors, including the number-one paper—"**Implosion dynamics** measurements at the National Ignition Facility." The other three are:

- "**Development** of the indirect-drive approach to inertial confinement fusion and the target physics basis for ignition and gain"
- "**Design** of a deuterium and tritium-ablator shock ignition target for the National Ignition Facility"
- "The **physics basis** for ignition using indirect-drive targets on the National Ignition Facility"

NATURE PAPER REPORTS FIRST-EVER MEASUREMENT OF SUPERMASSIVE BLACK HOLE SPIN RATE

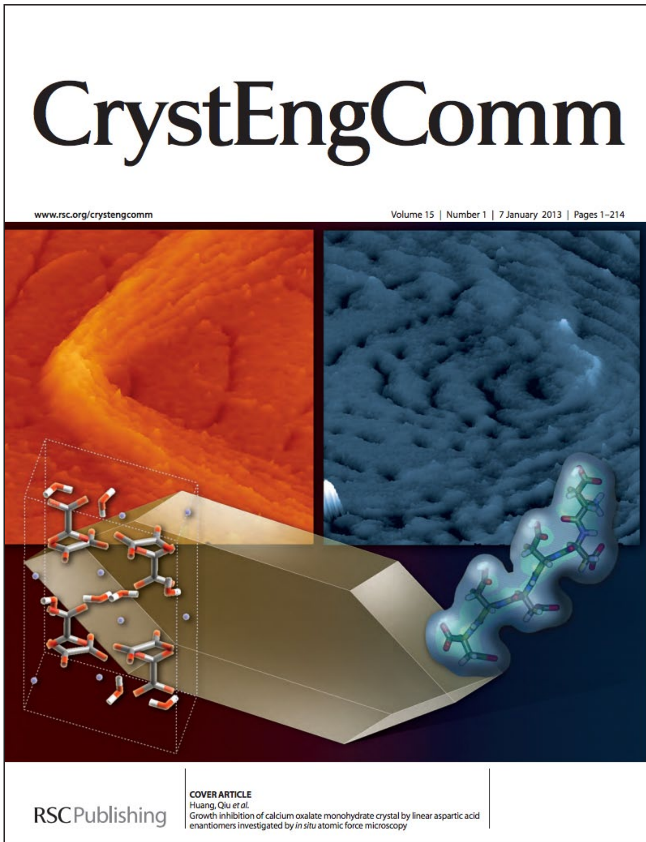


A Nature **paper** authored by an international team including LLNL astrophysicist and LDRD Program Director Bill Craig reports the first-ever definitive measurement of the spin rate of a supermassive black hole. The findings—made by the two x-ray space observatories, NASA's Nuclear Spectroscopic Telescope Array (**NuSTAR**) and the European Space Agency's XMM-Newton—solve a longstanding debate about similar measurements in other black holes. This knowledge about spin is important because, as the *Nature* "News and Views" **highlight** about the article explains, "our understanding of galaxy formation and evolution is intimately linked to our understanding of supermassive black holes. The energy released by a growing supermassive black hole can be so powerful that it disrupts the normal growth of the host galaxy." Says Bill, "We know that black holes have a strong link to their host galaxy. Measuring the spin, one of the few things we can directly measure from a black hole, will give us clues to understanding this fundamental relationship." Important optics design and testing work for NuSTAR was done at LLNL, where this x-ray-focusing technology dates back to the LDRD-supported High Energy Focusing Telescope (HEFT) instrument, the success of which allowed Livermore to propose NuSTAR to NASA. The figure (courtesy of NASA/JPL-Caltech) depicts two theories on how to interpret the iron "fingerprints" in a black hole's accretion disk. NuSTAR has enabled researchers to rule out the bottom theory in favor of the top one—known as the rotation model—in which iron is spread out by distortion effects caused by the black hole's immense gravity, which in turn allows inference of the black hole's spin rate from the amount of distortion observed in the iron.

WISE FINDS ITS FIRST DISTANT GALAXY CLUSTER

A multinational team including Livermore-affiliated Adam Stanford **published a paper** in *Astrophysical Journal Letters* announcing the first distant galaxy cluster discovered with NASA's Wide-field Infrared Survey Explorer (**WISE**). This galaxy cluster, dubbed MOO J2342.0+1301, is located more than 7 billion light years away—halfway back to the time of the Big Bang—and is hundreds of times more massive than our Milky Way. "By uncovering the most massive of galaxy clusters billions of light-years away with WISE, we can test theories of the universe's early inflation period," says Anthony Gonzalez of University of Florida, Gainesville, who led the research.

A BIOMINERALIZATION LOOK AT KIDNEY STONE COMPOUNDS



Kang Rae Cho—then a Lawrence Scholar and now a postdoc at LBNL—and others have **published a study** in *Crystal Engineering Communications* on using by linear acid enantiomers to inhibit the growth of crystals of calcium oxalate monohydrate (COM), the main inorganic component of kidney stones. The authors' work was also featured on the inside front cover of the journal. The in situ atomic force microscopy measurements that were central to this study were a collaborative effort among LLNL, LBNL, UCLA, and the University of South Alabama. The team examined morphological changes and measured kinetic effects on COM crystals grown in the presence of different stereoisomers of aspartic acid residues. The results support the idea that the macroscopic chiral symmetry of COM crystals grown in the presence of "foreign" chiral molecules is caused by differential stereochemical matching between the foreign molecules and symmetry-related features present on the surfaces of the growing COM crystals.

EXPERIMENTS POINT TO MORE-OXIDIZING CONDITIONS OF EARTH'S CORE FORMATION

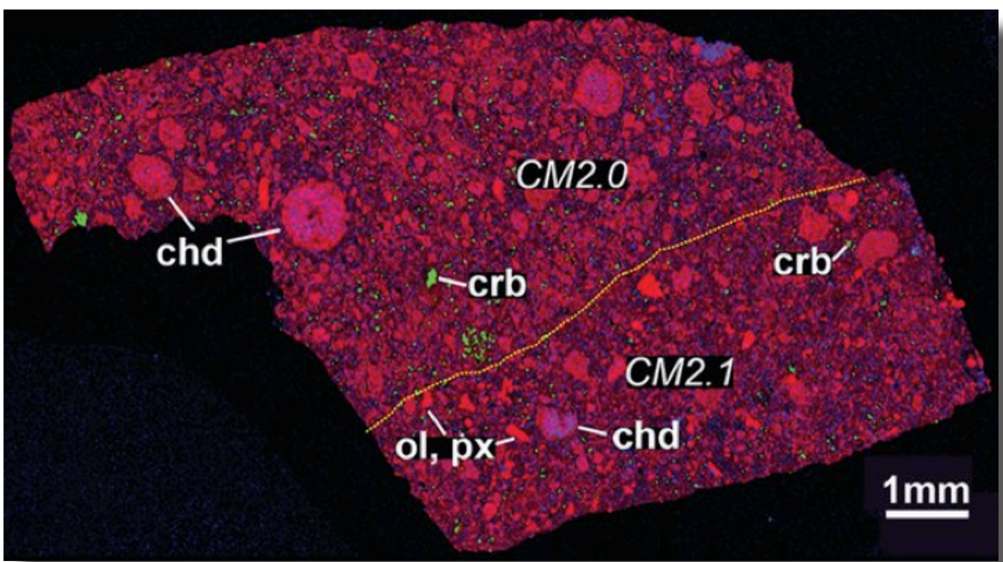
In a **paper published** in *Science*, a team including LLNL geophysicist Rick Ryerson published their conclusions of diamond anvil experiments—that the Earth's core formed under conditions much more oxidizing than previously believed. Although scientists know that the Earth accreted from some mixture of meteoritic material, no simple way exists to quantify the proportions of these various materials. The new research defines how various materials may have been distributed and transported in the early solar system. Through a series of laser-driven high-pressure and -temperature experiments, the team demonstrated that the distribution of siderophile elements—those combining readily with iron—is explained by core-formation conditions that are more oxidizing than previously predicted. Based on their results, the team proposes that Earth formed from oxidized materials—"We found," said Rick, "that planet accretion under oxidizing conditions is similar to those of the most common meteorites"—and that the subsequent transfer of oxygen from Earth's mantle to the core explains the present-day mantle's redox state. This conclusion also reconciles both observed concentrations of siderophile elements in the mantle and geophysical mechanisms limiting the presence of light elements in the core.

TEAM SOLVES LONGSTANDING MYSTERY ABOUT CERIUM

Led by LLNL scientist Magnus Lipp and former Livermore scientist Joseph Bradley, researchers at LLNL, the University of Washington, Stanford University, and the Carnegie Institute have answered a longstanding question about cerium, which undergoes a surprising, large isostructural volume collapse at high pressure. The LLNL team found an experimental signature that strongly favors one model for the collapse—Kondo volume collapse. The work **appears** in the November 9 edition of *Physical Review Letters*. "We have developed a very powerful methodology for studying rare earth systems at high pressure using x-ray spectroscopy," Joseph said. In collaboration with the University of Washington, the team has **developed instrumentation** that speeds up data collection by a factor of 100 or more. "This means that we can not only answer the cerium question, but we can study many systems and gain some real understanding about f electron delocalization in general, which is a 'holy grail' question in condensed matter physics," said Joe. "In other words, it is one that can be directly transferred to the 5f electron in actinides."

METEORITE ANALYSIS PUBLISHED IN *SCIENCE*

A consortium of scientists—including the Laboratory's Gary Eppich—that analyzed fragments of the Sutter's Mill meteorite, which landed in Coloma, California, on April 22, 2012, have **published their findings** in *Science*, in which they conclude that the meteorite belongs to the rare carbonaceous Mighei (CM) class of meteorites. More importantly, the researchers believe they have identified the point of origin of these relatively pristine samples of solids formed in the early solar system—the Eulalia asteroid family, which was recently proposed as a source of primitive C-class asteroids in orbits that pass Earth. The image is a combined elemental map of a sample containing extensively aqueously altered lithologies (CM2.0 and CM2.1), with a sharp boundary indicated by a yellow dashed line. Both lithologies contain chondrule pseudomorphs (chd) embedded in a phyllosilicate-rich matrix and abundant carbonate grains (crb), but only CM2.1 contains rare olivine (ol) and pyroxene (px) grains of incompletely hydrated chondrules and other formations.

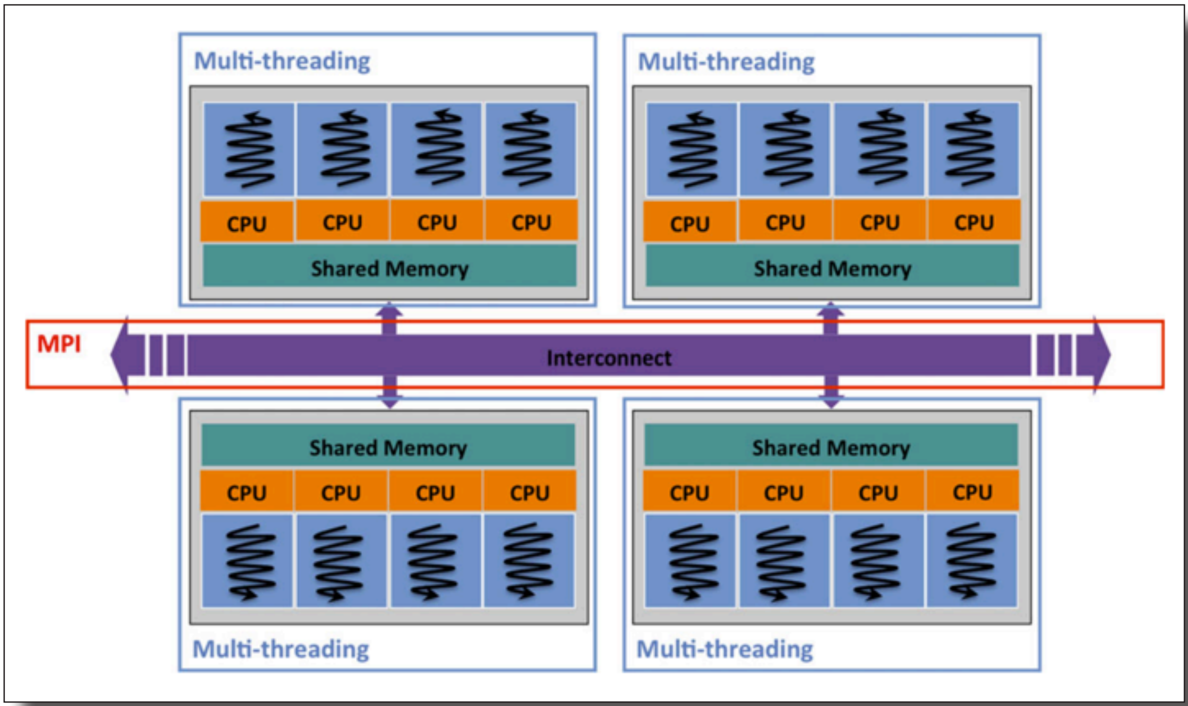


BIOLOGICAL FATE OF SILICA NANOPARTICLES UNCOVERED WITH AMS

In a **study published** in the October 17, 2012 edition of *Nanoletters*, LLNL researchers Mike Malfatti, Heather Palko, Ed Kuhn, and Ken Turteltaub report on accelerator mass spectrometry measurements used to investigate the relationship between administered dose, pharmacokinetics, and long-term biodistribution of silica nanoparticles. Because of unique properties such as monodispersity, large surface area, and high drug loading efficiency, silica nanoparticles have been developed for use in personal care products, some foods, and a vast array of biomedical uses, such as optical imaging, cancer therapy, targeted drug delivery, and controlled drug release—despite the lack of a clear, overarching understanding of their long-term biological effects. Pharmacokinetic analysis using carbon-14-labeled nanoparticles showed that they were rapidly cleared from the circulatory system and distributed to various body tissues, where they persisted over the 8-week duration of the study. This finding raises questions about the potential for bioaccumulation and associated long-term effects.

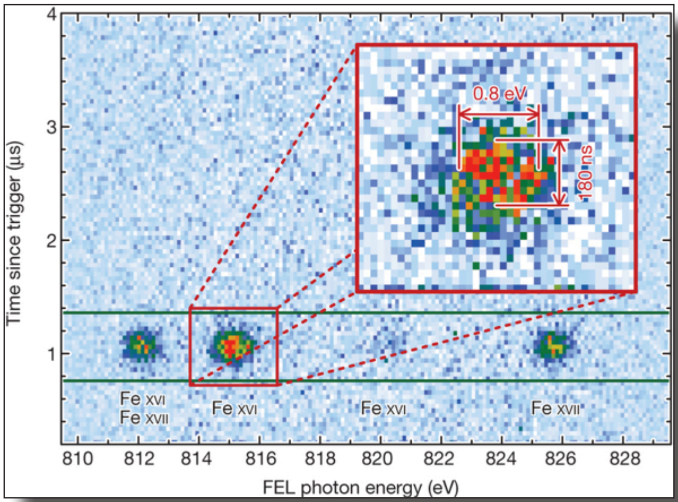
HYBRID APPROACH TO COMPUTATIONAL DRUG CANDIDATE SCREENING

A **paper** by Xiaohua Zhang, Sergio Wong, and Felice Lightstone published in the *Journal of Computational Chemistry* was also **highlighted** by the online high-performance computing news service HPC Wire. The authors report on a new hybrid scheme for computationally screening drug candidates using molecular docking, in which a set of small molecules of interest are evaluated according to how well they "fit" into and bind to an active site in a target protein molecule. The authors set their sights on solving two roadblocks to wider use of the technique—the serial, computationally intensive nature of the task, and problems in scaling codes to large high-performance computing platforms. The new paper reports on the development of their new hybrid scheme for parallelizing a molecular docking program that combines message passing interface and multithreading approaches. The LLNL team modified a popular open-source, PC-based docking program developed by Oleg Trott at the Scripps Research Institute to incorporate their new approach. The new code, called **VinaLC**, scales to more than 15,000 CPUs with a low overhead cost, with one million compound-docking calculations taking only 1.4 hours to finish. The performance of VinaLC therefore represents a dramatic improvement in the state of the art. The figure illustrates the mixed parallel scheme.



LCLS RESULTS NARROW DOWN CAUSE OF ASTROPHYSICAL OBSERVATION–MODEL MISMATCH

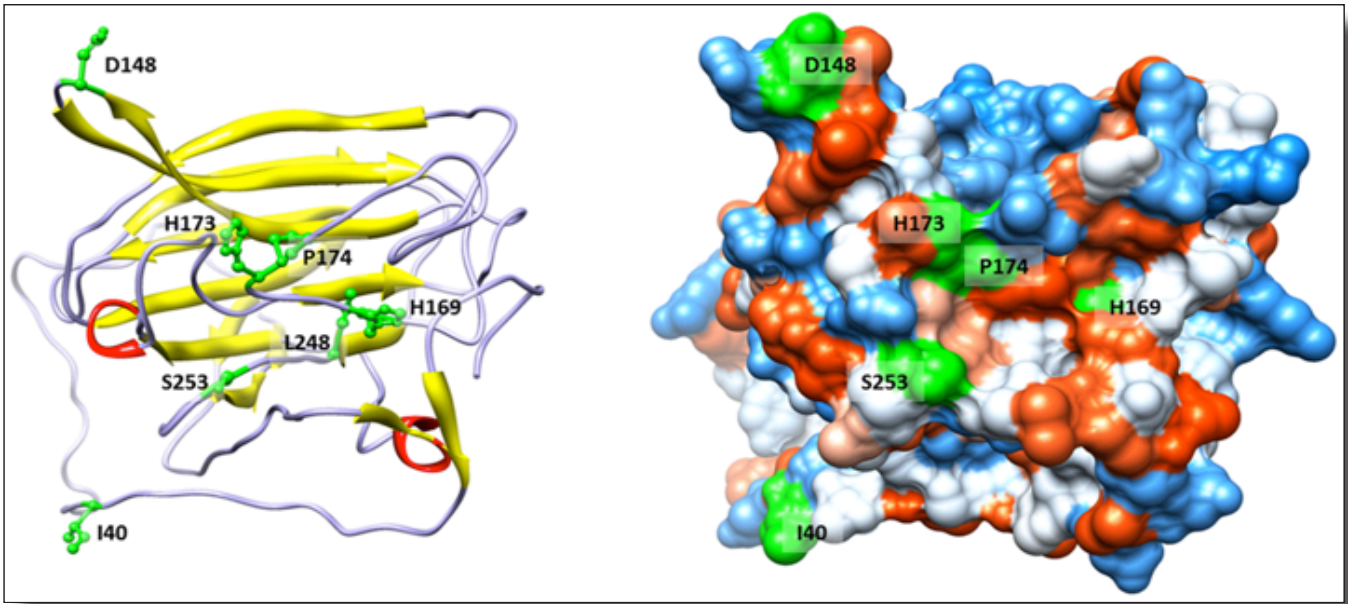
In a **paper** appearing in *Nature*, an international team of researchers including several from LLNL reports the results of an experiment in which iron ions were created and captured using an electron-beam ion trap (EBIT) and were then induced to fluoresce by subjecting them to femtosecond-duration x-ray pulses of the x-ray free-electron laser at the Linac Coherent Light Source. This experiment was the first ever to couple an EBIT to an x-ray laser and marks the opening of an entirely new venue for astrophysical research. The goal of the experiment was to isolate a key aspect of the quantum mechanical description of the line emission of highly ionized iron, which despite its importance in astrophysics does not have a well-described spectrum in even the best astrophysical models. This has affected the interpretation of observations by the Chandra and XMM-Newton orbiting x-ray missions. The team's EBIT measurements differed greatly from the best quantum mechanical calculations in a manner suggesting that poor agree-



ment between observations and current models is due to the quality of the atomic wave functions used to model the underlying atomic physics, rather than an insufficient representation of collisional processes. The figure graphs time coincidence between the free-electron laser pulse and detected x-ray fluorescence and demonstrates the efficiency of the latter's detection, which was the key to successful measurement.

INFECTION-ENABLING MUTATION IN RNA VIRUS PINPOINTED

In a **study published** in *PLoS ONE*, Lab researcher Monica Borucki and colleagues report on the genomic changes in a coronavirus as a result of multiple passages between human and bovine hosts. Their work is part of a larger effort to understand the specific mutations that allow such RNA viruses—which account for almost three-quarters of all emergent pathogens, including HIV and SARS—to infect their hosts. Monica et al. found that the genome of the final samples frequently contained a 12-nucleotide insert mutation, while extensive sequencing of the prepassage sample showed the mutation to be present but very rare in the initial population. They conclude that the mutation, which is likely to be key to interspecies transmission, was "selected" from a preexisting genome pool rather than developed through de novo mutation. The findings shed light on the role of genetic diversity in the "success" of RNA viruses. The figure shows two aspects of a structural model of the receptor binding domain from the bovine coronavirus studied—a ribbon representation (left) and hydrophobic surfaces (right). Colors of the hydrophobic surfaces range from blue for the most polar residues to white to orange–red for the most hydrophobic residues. Positions of nonsynonymous mutations are colored in green.



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Questions? Comments?

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